

The lattice gas model with isospin-dependent interactions

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Abstract

In this paper we continue the investigation of the lattice gas model. The main improvement is that we use two strengths for bonds: one between like particles and another between unlike particle to implement the isospin-dependence of nuclear force. The main effect is the elimination of unphysical clusters, like the dineutron or diproton. It is therefore a better description of nuclear system. Equation of state in mean field theory is obtained for nuclear matter as well as for $N \neq Z$ systems. Through numerical and analytical calculation we show that the new model maintains all the important features of the older model. We study the effect of the Coulomb interaction on multifragmentation of a compound system of $A=86$, $Z=40$ and also for $A=197$, $Z=79$. For the first case the Coulomb interaction has small effect. For the latter case the effect is much more pronounced but typical signatures of the lattice gas model such as a minimum (maximum) in the value of τ (S_2) are still obtained but at a much lower temperature.

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I. INTRODUCTION

Over the past a few years we have been developing a lattice gas model for the study of nuclear multifragmentation[1-5]. In this model n nucleons are placed in N cubes and they interact with nearest neighbour interactions. In most of this work the interaction between neutron-neutron, proton-proton and neutron-proton was taken to be identical although we have sometimes used[5] a more complicated model in which interactions between like particles are different from those between unlike particles. The purpose of this paper is to more fully expose this improved model and to examine its relationship with our earlier and simpler model. Among other things we will also show that the important conclusions reached with our simpler model go through in our improved version.

The lattice gas model has the attractive feature that it can provide an equation of state but it can also provide the cluster distribution. Most of the observables are calculated using Monte-Carlo simulations. We used Metropolis algorithm in our simulations. The n particles are distributed in N boxes according lattice gas Hamiltonian and their momenta are generated from Maxwell-Boltzmann distribution at a prescribed temperature. Calculation of clusters is straightforward. Two nucleons in neighbouring cells are part of the same cluster if the relative kinetic energy is less than the strength of the attractive bond: $p_r^2/2\mu + \epsilon < 0$. Here p_r is the relative momentum, μ the reduced mass and ϵ is negative(attractive interaction). This prescription is sufficient to calculate cluster distribution. The motivation for introducing two kinds of bond is now obvious. If the neutron-neutron bond or the proton-proton bond is attractive then each numerical simulation can generate dineutrons and diprotons which in reality do not exist in nature as composites. One can get rid of these unphysical clusters by simply making the neutron-neutron and proton-proton bonds zero or repulsive.

For completeness we mention some more features of the lattice gas model that were studied in [1,2]. One finds that at a certain temperature the distribution of composites is a power law: $Y(Z) \propto Z^{-\tau}$ where $Y(Z)$ is the number (averaged over many simulations) of

composites with Z protons. As is a common practice, we will extract a value of τ even when the distribution has significantly deviated from a power law[6]. This value is extracted by using

$$\frac{\sum_2^{10} ZY(Z)}{\sum_2^{10} Y(Z)} = \frac{\sum_2^{10} ZZ^{-\tau}}{\sum_2^{10} Z^{-\tau}} \quad (1.1)$$

We also calculate the second moment $S_2 = \sum' A^2 Y(A)/n$ where in the sum the largest cluster is excluded. The usefulness of S_2 was emphasized by Campi[7]. Since the lattice gas model has a Hamiltonian, its average energy at any temperature can be calculated. The excitation energy and specific heat C_v per particle can be calculated. We will find this useful too.

II. THE EQUATION OF STATE

We have N boxes in the lattice in which we have to put n_n neutrons and n_p protons; $n_p + n_n = n < N$; $n/N = V_0/V = \rho/\rho_0$ where V_0, ρ_0 are normal nuclear volume and density respectively. In principle, we can have three kinds of bonds: $\epsilon_{nn}, \epsilon_{pp}$ and ϵ_{pn} . In the most general case where these interactions can take any arbitrary values a rich assortment of phenomena is predicted. The grand canonical partition function of this general lattice gas model can be mapped on to a spin 1 Ising type model in the presence of a magnetic and quadrupole field. These have been studied in detail in the past[8]. For the nuclear case the values of the interactions are quite restricted and the richness of phenomena disappears. First of all we have to set ϵ_{nn} and ϵ_{pp} to be either zero or repulsive so that one avoids producing unphysical dineutron or diproton bound clusters. Charge independence of nuclear forces suggests that we put $\epsilon_{nn} = \epsilon_{pp}$. From now on we will write ϵ_{pp} for both ϵ_{pp} and ϵ_{nn} . In our past work[5] and also in other modelings[9] of nuclear collisions using classical mechanics a slightly repulsive ϵ_{pp} was used. To avoid proliferation of parameters we will set this bond to zero in this work. The binding energy of nuclear matter fixes the value of ϵ_{pn} at -5.33 MeV.

Throughout this work γ stands for the number of nearest neighbours. In 3 dimensions one has $\gamma = 6$. We use the Bragg-Williams mean field theory using the canonical ensemble.

There are N boxes and n_p protons and n_n neutrons. Let one of the boxes be occupied by a proton. Then, in the Bragg-Williams approximation, among its nearest neighbours, on the average $\gamma n_p/N$ will be occupied by protons and $\gamma n_n/N$ by neutrons. The number of $n-p$ bonds will be $\gamma n_p n_n/N$, the number of $p-p$ bonds will be $(1/2)\gamma n_p n_p/N$ where the factor of $1/2$ remedies the double counting for proton-proton bonds. Similarly starting with a box occupied by a neutron we come up with the same number of neutron-proton bonds and the number of neutron-neutron bonds is determined to be $(1/2)\gamma n_n n_n/N$. Thus the interaction energy when there are n_p protons, n_n neutrons placed in N boxes is $E = \gamma(\epsilon_{pn}n_p n_n + \epsilon_{nn}(n_n^2 + n_p^2)/2)/N$ and the partition function is

$$Z(N, n_p, n_n) = \frac{N!}{(N - n_p - n_n)!n_p!n_n!} \exp(-\beta E) \quad (2.1)$$

We now find pressure P from the equation $P = kT[\partial \ln Z / \partial V]_T$ and $V = a^3 N$ where $a^3 = 1/\rho_0$ is the volume of each box. Using Stirling's formula one arrives at

$$P = \rho_0 kT \ln \frac{N}{N - n} + \rho_0 \gamma \epsilon_{pn} (n_p/N)(n_n/N) + \rho_0 \gamma \epsilon_{nn} ((n_n/N)^2 + (n_p/N)^2)/2 \quad (2.2)$$

Introduce an asymmetry parameter $\eta = (n_n - n_p)/(n_n + n_p)$ which takes value 1 for neutron matter, 0 for nuclear matter and -1 for proton matter. We can then write

$$P = \rho_0 kT \ln \frac{V}{V - V_0} + \frac{1}{2} \rho_0 \gamma \frac{V_0^2}{V^2} \left[\frac{\epsilon_{pn} + \epsilon_{nn}}{2} + \frac{1}{2} \eta^2 (\epsilon_{nn} - \epsilon_{pn}) \right] \quad (2.3)$$

Determine the critical point from $\partial P / \partial \rho = \partial^2 P / \partial \rho^2 = 0$. This gives the critical density $\rho_c = .5\rho_0$ and the critical temperature to be $-(\gamma/4)[(\epsilon_{pn} + \epsilon_{pp})/2 + (1/2)\eta^2(\epsilon_{nn} - \epsilon_{pn})]$. In this approximation with ϵ_{pn} attractive and $\epsilon_{nn} = 0$ the critical temperature for nuclear matter (which has $\eta=0$) would be highest at $-(\gamma/4)(\epsilon_{pn}/2)$ and would fall off quadratically with η to 0 at neutron or proton matter.

The Bragg-Williams approximation is the simplest mean-field approximation. An improved treatment using Bethe-Peierls approximation is worked out in the appendix. The mean field calculation shown in this section and the appendix is merely to form a rough idea about the nature of phase transition. In practical calculations we need to obtain the

yields of the composites at a given temperature. Mean field theories do not provide these and we need to do event by event calculation which can be obtained through Monte-Carlo samplings.

III. MONTE-CARLO RESULTS

As far as we know exact results with two kinds of bonds are not available. For one kind of bond one can often interpret essentially exact although numerical results from well-studied spin 1/2 Ising model for use in the lattice gas model. In the absence of such exact results our only recourse is to compare numerical results obtained with two kinds of bonds, i.e., $\epsilon_{pn} = -5.33$ MeV, $\epsilon_{nn} = 0$ with those obtained with one kind of bond that we have used before, i.e., $\epsilon_{pn} = \epsilon_{nn} = -5.33$ MeV. We use here $N = 7^3$, which is a number appropriate for finite systems that we will investigate. As mentioned in the introduction the calculation proceeds by first putting the required number of protons and neutrons in the N boxes using a standard Metropolis algorithm. Nucleons are then assigned momenta from Monte-Carlo sampling of a Boltzmann distribution at the given temperature. The energy of the event can now be calculated. Clusters are then determined as explained in the introduction. The results shown in Figs. 1 and 2 are obtained by averaging over 1000 events for selected temperatures. For two assumed freeze-out densities we calculate the specific heat, the second moment S_2 and the deduced values of τ . The unit chosen in the graph for temperature is $T_c = 1.1275|\epsilon_{pn}|$ which is the T_c for an infinitely large lattice with one kind of bond. We find that the peaking of C_v, S_2 and the minimum of τ happen at a slightly lower temperature (about ten percent) with two kinds of bond as compared to when the same bond is used for all the particles. For example for the minimum of τ to appear at the same temperature the value of $\epsilon_{pp} = \epsilon_{pn}$ has to be set at about 10% lower value than the value of ϵ_{pn} when ϵ_{pp} is set to zero. Qualitatively and even semi-quantitatively the results in the two models look similar when this renormalisation of the strength is done. However, the peaking of C_v is more pronounced in the two bonds model.

All models which employ freeze-out densities assume that the freeze-out density is less than $.5\rho_0$. If the freeze-out density is less than $.5\rho_0$ then in the lattice gas model a peak in the C_v will signify the crossing of the co-existence curve and a first order phase transition. The value of specific heat can be deduced from the caloric curve [10] but locating the peak is very difficult in experiment. In a recent paper we have suggested[11] that since the peaking of C_v is accompanied by a minimum in τ and a maximum in S_2 , the appearance of the last two could be taken as a signal of the phase transition. The appearance of the maxima in S_2 and of the minimum in τ in close vicinity of the maximum in C_v happens in both the versions of the lattice gas model.

IV. A STUDY ON THE EFFECTS OF THE COULOMB FORCE

Here we follow the methods employed in ref [3]. At that time we studied the influence of the Coulomb force on fragmentation of a system which had 85 nucleons and found the effects to be small. For a much larger system (Au on Au: central collision so that the compound system has $A \approx 394$) we found the effect to be very large. One of the rather unavoidable features of the lattice gas model is the appearance of a minimum in the extracted value of τ as a function of temperature. This feature disappeared for the very large system of $A = 394$ because of the Coulomb interaction.

For completeness a short description of a similar calculation but done for two kinds of bonds will be given here. In addition to lattice gas calculations, we do molecular dynamics calculations whose purpose is two-fold. One is to check if the predictions of a lattice gas model can resemble those of a molecular dynamics calculation provided the initial conditions are the same and the forces are chosen to be such that they resemble implied forces of the lattice gas model. For this we place the n_p protons and n_n neutrons in the N boxes using as usual Metropolis algorithm. Next we assign the momenta from Monte-Carlo sampling of a Maxwell-Boltzmann distribution. Once this is done the lattice gas model immediately gives the cluster distribution using the rule that two nucleons are part of the same cluster

if $p_r^2/2\mu + \epsilon < 0$. To calculate clusters using molecular dynamics we propagate the particles from this initial configuration for a long time under the influence of the chosen force (we will give the force parameters shortly). At asymptotic times the clusters are easily recognised (a detailed discussion of cluster recognition which requires shorter computer times can be found in ref 12). The cluster distribution in the two models can now be compared. Fig. 3 shows the two prescriptions give nearly the same answer.

We now come to the second and more important purpose of the molecular dynamics calculation. We now add the Coulomb interaction to the nuclear part. The initialisation of putting the nucleons in N boxes is done again but now with the inclusion of Coulomb forces. We then do a molecular dynamics propagation including the Coulomb force. The clusters can again be calculated and compared with the cases where the Coulomb force was ignored.

We now give the force parameters for molecular dynamics propagation. The neutron-proton potential was taken to be $v_{pn}(r) = A[B(r_0/r)^p - (r_0/r)^q] \exp([1/(r/r_0 - a)])$ for $r/r_0 < a$ and $v_{pn}(r) = 0$ for $r/r_0 > a$. Here $r_0 = 1.842$ fm is the distance between the centers of two adjacent cubes. We have chosen $p = 2, q = 1, a = 1.3, B = .924$ and $A = 1966$ MeV. With these parameters the potential is minimum at r_0 with the value -5.33 MeV, is zero when the nucleons are more than $1.3r_0$ apart and becomes strongly repulsive when r is significantly less than r_0 . We now turn to the nuclear part of like particle interactions. Although we take $\epsilon_{pp} = 0$ in lattice gas calculations the fact that we do not put two like particles in the same cube would suggest that there is short range repulsion between them. We have taken the nuclear force between two like particles to be the same expression as above plus 5.33 MeV upto $r = 1.842$ and zero afterwards: $v_{pp}(r) = v_{pn}(r) - v_{pn}(r_0)$ for $r < r_0$ and 0 afterwards. This means there is a repulsive core which goes to zero at r_0 and is zero afterwards.

The results shown in Figs. 3 and 4 can be summarised as follows. Fig 3. first of all shows that if there is no Coulomb interaction then lattice gas model results are quite close to that of molecular dynamics simulation provided in the latter one starts from the same initial condition and uses a force suitably chosen. Fig 3 also shows that in the case of

$A = 85, Z = 40$ the Coulomb force does not have a large effect. The minimum in τ and the maximum in S_2 are shifted to slightly lower temperature. The effect for $A = 197, Z = 79$ is much bigger. The minimum in τ and the maximum in S_2 are shifted from 4.8 MeV (lattice gas without Coulomb) to about 2.4 MeV. Our previous calculation showed that there is no minimum in τ for $A = 394, Z = 158$. So somewhere between these two limits the minimum will vanish.

V. DISCUSSION

The two bond model is a natural progression of the simpler lattice gas model. In this paper we have done calculations with the two bond model. Although in detail the two models differ the major characteristics of the well studied simple model remain unchanged. The lattice gas model remains a quick tool to calculate experimental data.

When the Coulomb force is very strong the lattice gas model can not be relied upon. Figs. 3 and 4 give some indication of the reliability of the model in the presence of a Coulomb force. Calculations above indicate that a viable (although much more time consuming) prescription might be: obtain the initial conditions as in a lattice gas model. Put n nucleons in N boxes by Metropolis sampling where one includes in addition to lattice gas Hamiltonian the Coulomb force. Obtain momenta of each nucleon from a Monte-Carlo sampling of a Maxwell-Boltzmann distribution. Then propagate by molecular dynamics to obtain cluster distributions. Techniques developed in ref. 12 might be useful so that one does not need to run molecular dynamics till asymptotic times. One attractive feature of this hybrid model is that the Coulomb force is operative even during the formation of clusters as opposed to other models where the Coulomb force only adds repulsion between the composites already formed.

VI. ACKNOWLEDGEMENTS

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APPENDIX A:

We follow the method of reference 1. We break up the lattices into $N/(\gamma + 1)$ blocks, each of which contains 1 central box and γ nearest neighbours to it. We refer to Fig A.1 where for simplicity a two-dimensional lattice is shown. The interactions within each block are taken into account exactly while the interactions between different blocks are treated in an approximate fashion. The grand partition function can be written as the product of the grand partition functions of the $N/(\gamma + 1)$ blocks:

$$Z_{gr} = z_{gr}(block1)z_{gr}(block2).....z_{gr}(block\frac{N}{\gamma + 1}) \quad (A1)$$

We want to write down the grand partition function of the block denoted by 1,2,3, γ and 5. In the general case there will be two absolute fugacities λ_p and λ_n , the first referring to protons and the second to neutrons. The grand partition function for a block can be written as

$$z_{gr} = A + B + C \quad (A2)$$

where

$$A = (1 + e^{\lambda_p - \beta \bar{\epsilon}_p} + e^{\lambda_n - \beta \bar{\epsilon}_n})^\gamma \quad (A3)$$

$$B = e^{\lambda_p} (1 + e^{\lambda_p - \beta \bar{\epsilon}_p - \beta \epsilon_{pp}} + e^{\lambda_n - \beta \bar{\epsilon}_n - \beta \epsilon_{pn}})^\gamma \quad (A4)$$

$$C = e^{\lambda_n} (1 + e^{\lambda_p - \beta \bar{\epsilon}_p - \beta \epsilon_{pn}} + e^{\lambda_n - \beta \bar{\epsilon}_n - \beta \epsilon_{pp}})^\gamma \quad (A5)$$

Here A =contribution to the partition function when the central (innermost) site is empty, B =contribution to the partition function when the central site has a proton and C =contribution to the partition function when the central site has a neutron. Equation (4) takes the place of eq.(3.9) in ref [1]. The two constants $\bar{\epsilon}_p$ and $\bar{\epsilon}_n$ are the average interaction energy with the adjacent block when a proton (neutron) occupies a peripheral site.

The probability that the central site is occupied by a proton is n_p/N . Thus we have

$$\frac{n_p}{N} = \frac{B}{z_{gr}} \quad (\text{A6})$$

But since no particular site is favoured over another one, the average occupation of one of the peripheral sites must also be n_p/N . This gives

$$\frac{n_p}{N} = \frac{E + F + G}{z_{gr}} \quad (\text{A7})$$

where

$$E = e^{\lambda_p - \beta \bar{\epsilon}_p} (1 + e^{\lambda_p - \beta \bar{\epsilon}_p} + e^{\lambda_n - \beta \bar{\epsilon}_n})^{\gamma-1} \quad (\text{A8})$$

$$F = e^{\lambda_p} e^{\lambda_p - \beta \bar{\epsilon}_p - \beta \epsilon_{pp}} (1 + e^{\lambda_p - \beta \bar{\epsilon}_p - \beta \epsilon_{pp}} + e^{\lambda_n - \beta \bar{\epsilon}_n - \beta \epsilon_{pn}})^{\gamma-1} \quad (\text{A9})$$

$$G = e^{\lambda_n} e^{\lambda_p - \beta \bar{\epsilon}_p - \beta \epsilon_{pn}} (1 + e^{\lambda_p - \beta \bar{\epsilon}_p - \beta \epsilon_{pn}} + e^{\lambda_n - \beta \bar{\epsilon}_n - \beta \epsilon_{pp}})^{\gamma-1} \quad (\text{A10})$$

Similarly two equations can be written for n_n/N .

$$\frac{n_n}{N} = \frac{C}{z_{gr}} \quad (\text{A11})$$

$$\frac{n_n}{N} = \frac{I + J + K}{z_{gr}} \quad (\text{A12})$$

where I, J, K can be written down from expressions E, F, G by interchanging protons with neutrons.

Equations (8),(9),(13)and (14) determine the four constants $\lambda_p, \lambda_n, \bar{\epsilon}_p, \bar{\epsilon}_n$.

For $n_p = n_n$, the calculations simplify. Now we have $\lambda = \lambda_n = \lambda_p$ and $\bar{\epsilon} = \bar{\epsilon}_n = \bar{\epsilon}_p$. Then $B = E + F + G$ (eqs(8) and (9)) leads to

$$e^\lambda (1 + Q e^{\lambda - \beta \bar{\epsilon}})^{\gamma-1} = e^{\lambda - \beta \bar{\epsilon}} (1 + 2e^{\lambda - \beta \bar{\epsilon}})^{\gamma-1} + e^{2\lambda} (1 + Q e^{\lambda - \beta \bar{\epsilon}})^{\gamma-1} e^{\beta \bar{\epsilon}} Q \quad (\text{A13})$$

where we have defined $Q = e^{-\beta \epsilon_{pp}} + e^{-\beta \epsilon_{pn}}$. Dividing both sides of eqn (15) by $e^\lambda (1 + Q e^{\lambda - \beta \bar{\epsilon}})^{\gamma-1}$ we obtain

$$1 = e^{-\beta \bar{\epsilon}} \left(\frac{1 + 2e^{\lambda - \beta \bar{\epsilon}}}{1 + Q e^{\lambda - \beta \bar{\epsilon}}} \right)^{\gamma-1} \quad (\text{A14})$$

Rewrite eq.(8) as $2N/n = z_{gr}/B$ where $n = n_p + n_n$ to obtain

$$\frac{2N}{n} = 2 + e^{-\lambda} \left(\frac{1 + 2e^{\lambda - \beta\bar{\epsilon}}}{1 + Qe^{\lambda - \beta\bar{\epsilon}}} \right)^\gamma \quad (\text{A15})$$

Using eq(15) the above relation leads to

$$e^\lambda = \frac{n}{2(N - n)} e^{\beta\bar{\epsilon}\gamma/(\gamma-1)} \quad (\text{A16})$$

Define $x = e^{-\beta\bar{\epsilon}/(\gamma-1)}$. Going back to eq(17) one can now derive a simple solution for x :

$$x = \frac{1}{2} \left[\frac{N - 2n}{N - n} + \sqrt{\left(\frac{N - 2n}{N - n} \right)^2 + 2Q \frac{n}{N - n}} \right] \quad (\text{A17})$$

Values of $\bar{\epsilon}$ and e^λ from the definition of x and eq.(18).

Let us now go back to the partition function for the lattice as given by eq.(3). where it is written as a product of the partition functions of the $N/(\gamma + 1)$ blocks. If we simply z_{gr} for each little block as calculated above we will count twice the interaction between neighbouring sites in different blocks. For example, the binding energy between 1 and 6 (Fig. A.1) is included in $z_{gr}(\text{block 1})$ and it is included again in $z_{gr}(\text{block 2})$. We note that on the average there are n/N particles at each site and each block has γ peripheral sites. Thus when we evaluate the partition function for the lattice, the partition function for each block should be corrected by the multiplicative factor

$$\text{correction} = e^{\frac{1}{2}\beta\bar{\epsilon}\gamma n/N} \quad (\text{A18})$$

We can now use $PV = kT \ln Z_{gr}$, $V = N/\rho_0$, and $\ln Z_{gr} = N/(\gamma + 1) \ln z_{gr}$ to obtain

$$P = \rho_0 kT \frac{1}{\gamma + 1} \ln z_{gr} \quad (\text{A19})$$

where z_{gr} includes the correction factor.

In Fig. A2 we have drawn $P - V$ diagrams for nuclear matter for two cases: (1) $\epsilon_{pn} = \epsilon_{pp} = -5.33$ MeV and (2) $\epsilon_{pn} = -5.33$ MeV and $\epsilon_{pp} = 0$ MeV. In Bethe-Peierls approximation the T_c in the former case appears to be between 6 and 8 MeV and in the second case between 4 and 6 MeV.

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FIGURES

FIG. 1. A comparison of the calculated values of τ , C_v and the second moment S_2 in the one type of bond model (top panel) and two types of bonds model (bottom panel). Here as elsewhere $T_c \equiv 1.1275|\epsilon_{pn}| \approx 6$ MeV. The compound system has $A=103, Z=45$. Notice the maxima and the minimum shift to lower temperature when ϵ_{pp} is set to zero. Also C_v is more sharply peaked.

FIG. 2. The same as above except that a higher freeze-out density is used. The number of lattice sites is still 7^3 . Here $A=171, Z=70$.

FIG. 3. The top part compares the τ values extracted from a lattice gas calculation (dotted curve) with those extracted from a molecular dynamics calculation which had no Coulomb (dashed curve) and one which had Coulomb included in the molecular dynamics calculation (solid curve). Molecular dynamics without Coulomb gives results very similar to those of the lattice gas model. Here the effect of the Coulomb is small. The number of protons was 45. The lower part compares the second moments.

FIG. 4. Effect of Coulomb on τ and the second moment for a much larger system; $A=197, Z=79$. The minimum in τ and the maximum in S_2 shift from about 5 MeV to 2.4 MeV because of Coulomb effect. At some larger Coulomb field the minimum in τ will finally disappear.

FIG. A1. A square lattice is divided into blocks to illustrate the Bethe-Peierls approximation. See text for details.

FIG. A2. p-V diagram in the Bethe-peierls approximation with same bond strength -5.33 MeV (top panel) between all particles and for the case where we distinguish between like particle interaction and unlike particle interaction (bottom panel).

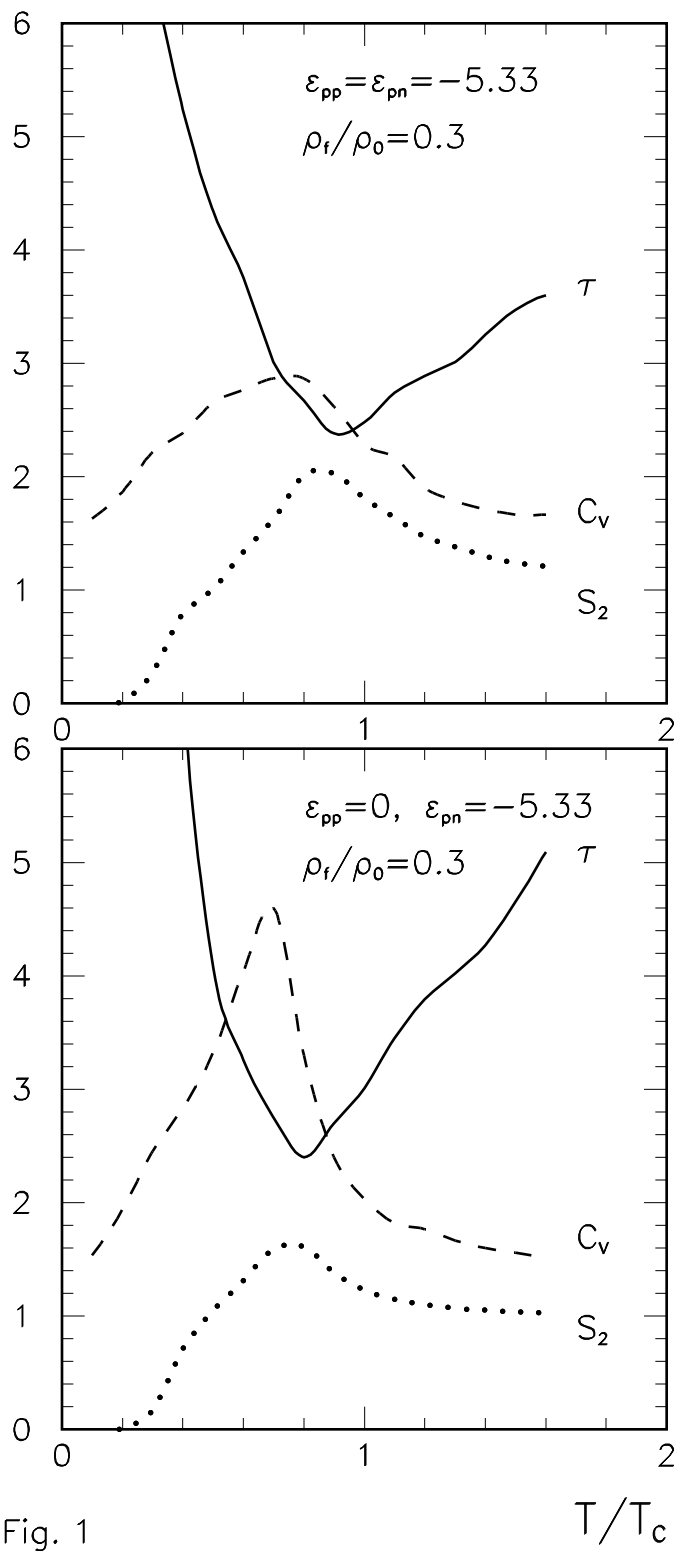


Fig. 1

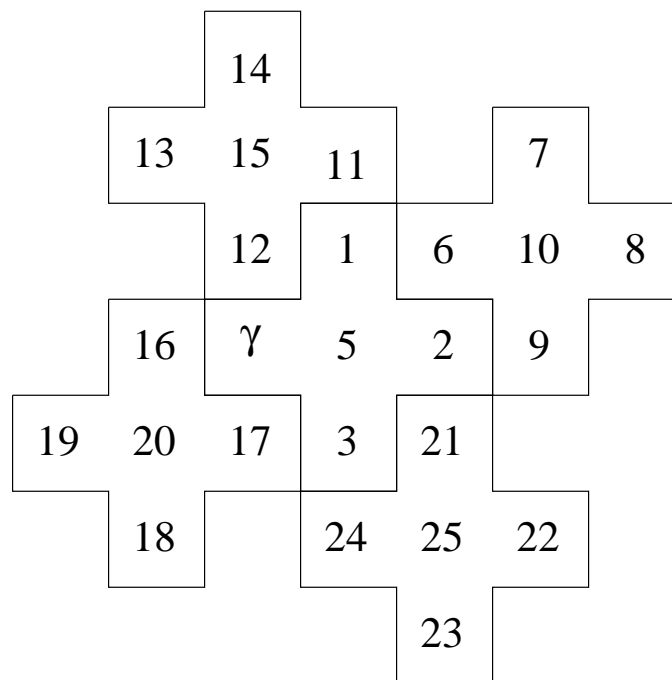


Fig. A1

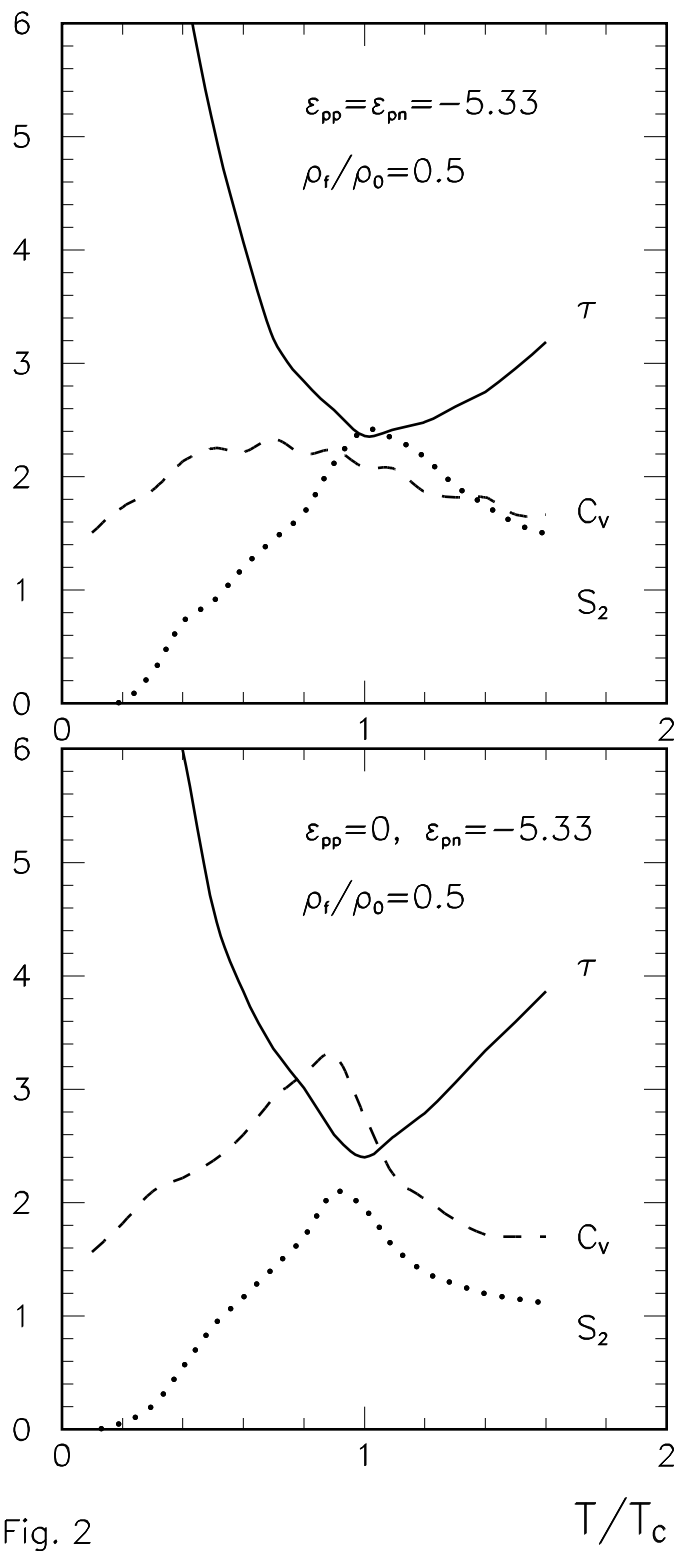


Fig. 2

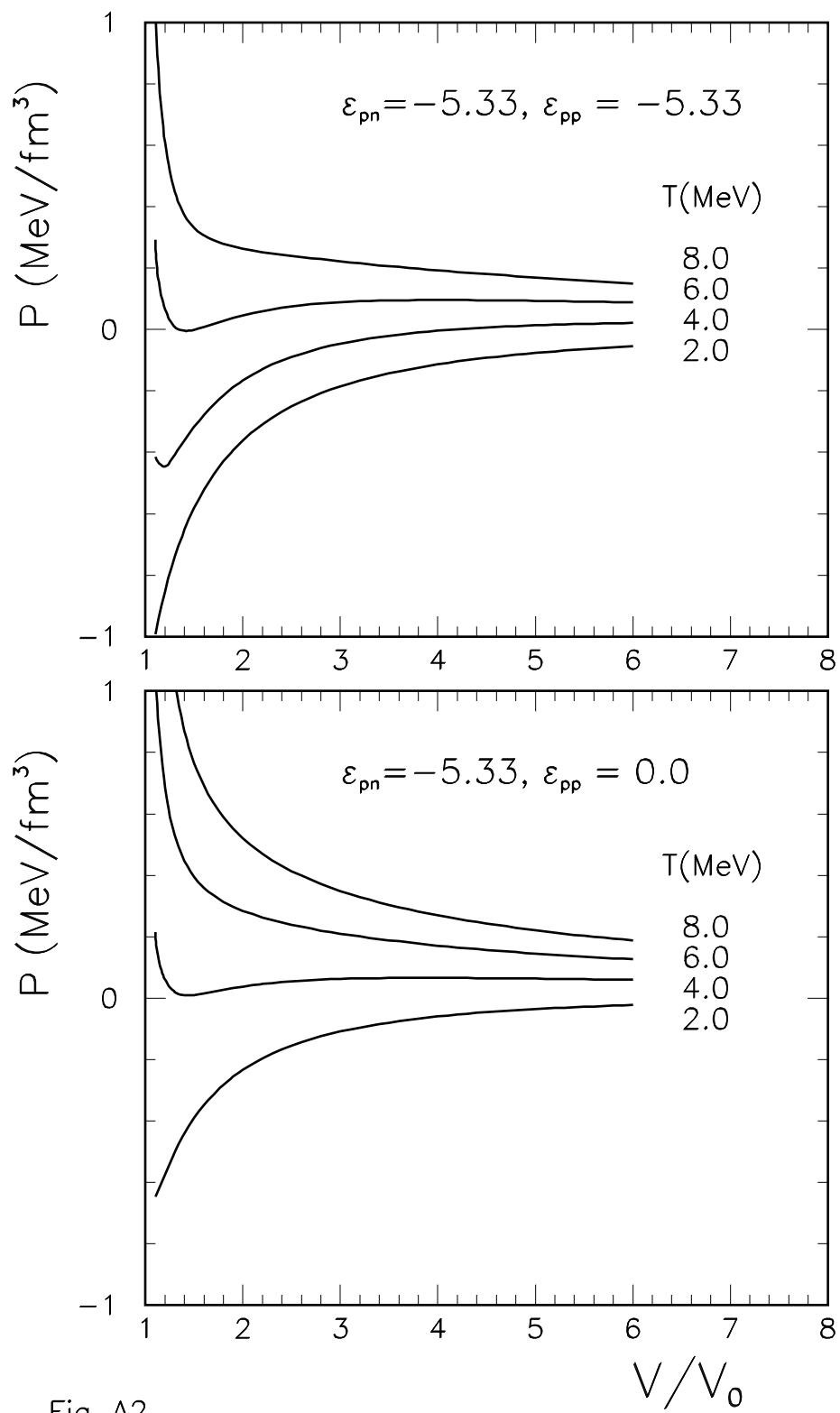


Fig. A2

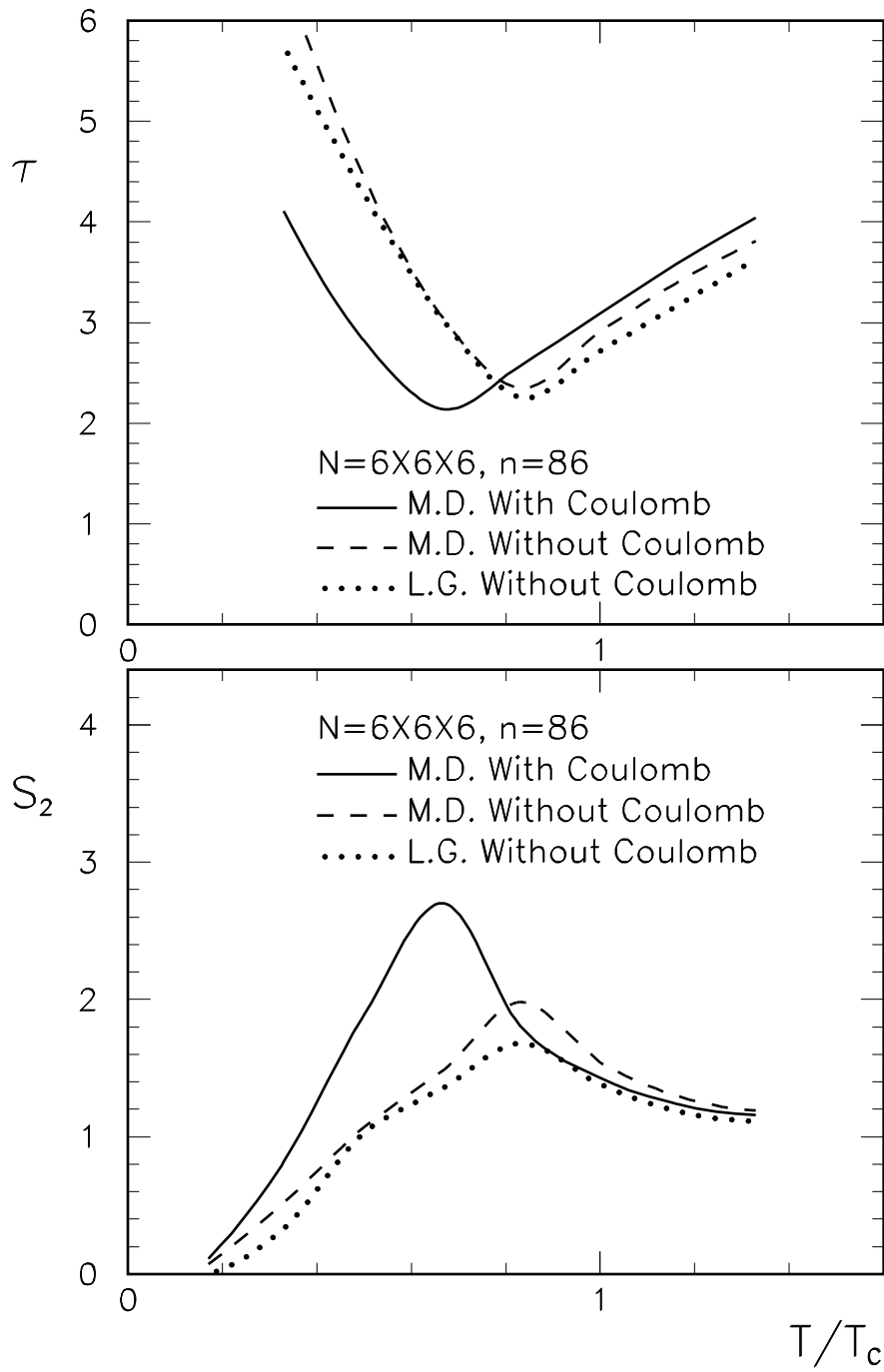


Fig. 3

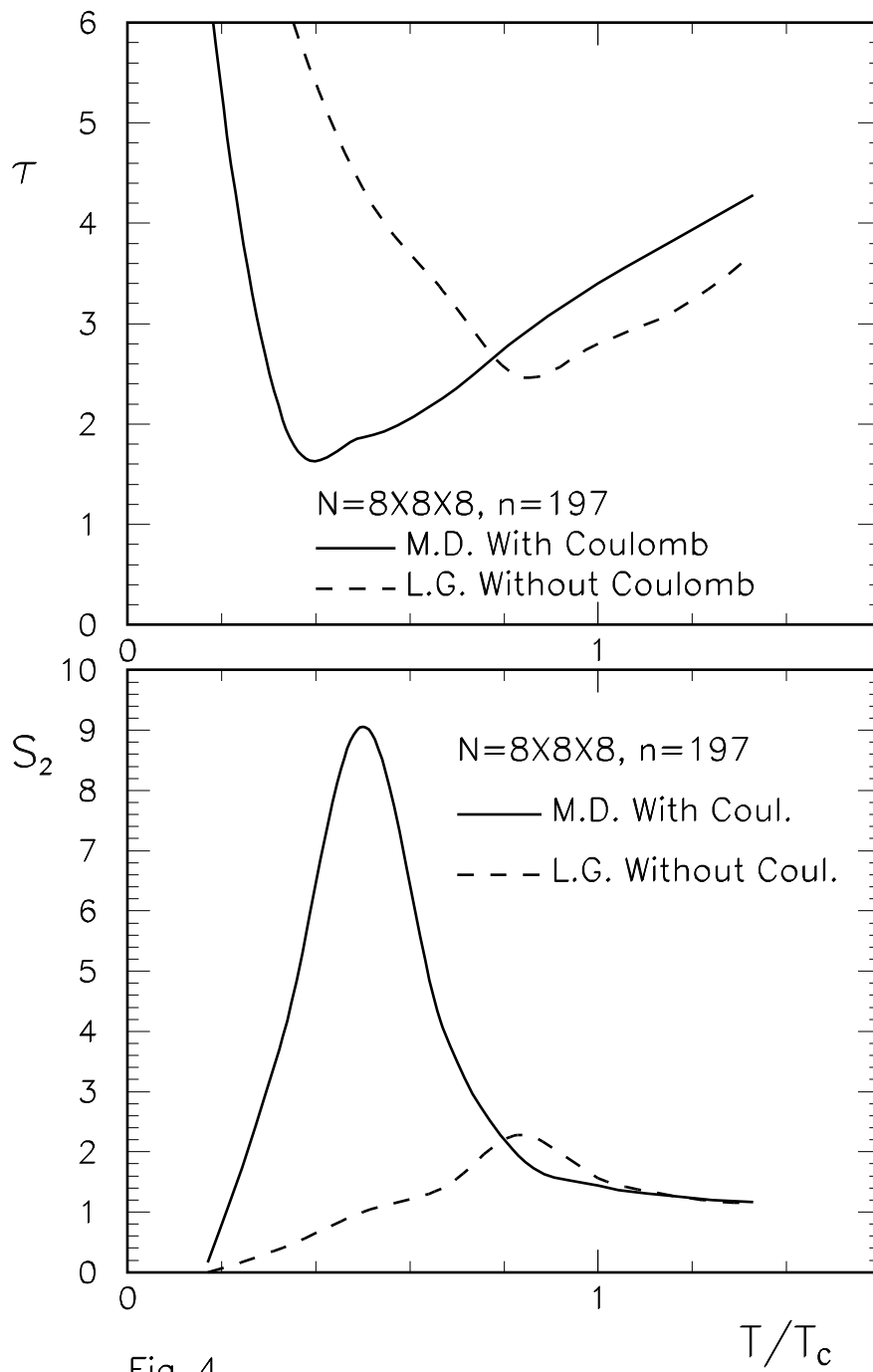


Fig. 4